Data Management and Domain Adjusting Strategies for Implementing Parallel SPH Method in JPUE Simulation

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Abstract

This paper presents a parallel implementation of smoothed particle hydrodynamics (SPH) method using the message passing interface (MPI) standard to simulate a turbulent jet or plume which is ejected from a nozzle into a uniform environment(JPUE). Background grid is used to reduce neighbors searching cost and decompose (redecompose) the domain. Space Filing Curve(SFC) based index is adopted to assign an unique identifier to each background grid. As simulation of JUPE requires adding of new particles during simulation, time-dependent SFC based indexes are assigned to particles to guarantee uniqueness of identifiers. Both particle and background grid are managed by hashtables which ensures quick and flexible accessing, adding and deleting of element. Additional link list attached to the hashtable is used to handle hash confliction. A SFC based three dimensional domain decomposition and a dynamic load balancing strategy are implemented to ensure good load balance. In addition, computational domain is adjusted during simulation to reduce computational cost. These strategies can be further applied to many other implementations of meshfree methods, especially those implemetations that require flexible accessing, adding and deleting of particles and backgroud grids.

1. Introduction

SPH is a meshless scheme, initially developed for astrophysical applications by Lucy [1] and Gingold and Monaghan [2]. Subsequently it was extended to large strain solid mechanics and computational fluid mechanics. A lot of research has been done in parallellization of SPH. Goozee [3] implemented a simple SPH code using MPI, OpenMP and BSP. Chen Wenbo [4] presented a parallel SPH implementation on multi-core CPUs. David W. Holmes [5] presented a simulation framework that enables distributed numerical computing in multi-core shared-memory environments. Domnguez [6] presented optimizations for both CPU and GPU parallelization of a SPH method. Angela Ferrari [7] parallelized a 3D SPH code using the message passing interface (MPI) standard, together with a dynamic load balancing strategy to improve the computational efficiency of the scheme. D. Kumar and Abani [8] implemented CPU parallel Godunov SPH in simulation of granular flows. A.J.C. Crespo [9] used the parallel power computing of GPUs to accelerate DualSPHysics by up to two orders of magnitude compared to the performance of the serial version.

However, most implementation of parallel SPH method is limited to bechmark problems like dam break, or relative simple scenarios like breaking-waves, floodings ect. Rare work has been done in simulation of more complicated problems, such as eruption of volcano plume which is essentially a mutilple phases, turbulent, ejection mixing process accompanied by microphysics phenomena like phase change of water, aggregation, reaction ect. Prediction of such more complicated phenomena with acceptable accuracy at given time window can not been acomplished without parallel computing. What's more, imposing of some types of boundary conditions (such as realistic wind feild, eruption boundary condition) requires dynamiclly adding and removing of particles during simulation. This requies efficient and more flexible data management scheme. What need to point out is that the benefit of flexible data management strategies are not only limited to specific implementations of SPH. Actually, flexibility in data management are more desperately needed in some advanced techniques of SPH, such as dynamic particle splitting techniques

[10], [11], which will give greater resolution at the area of interest by spliiting one large particle to several smaller ones. In this paper, we implement SPH to simulate a simplified version of complicated volcanic plume: the JPUE, and develop data management schemes for it.
Among existing CPU parallel SPH schemes, most of them focus on neighbors searching algorithm and dynamic load balancing. (eg. [7], [9]). Less attention has been paid to developing of more flexible data management schemes for more complicated problems. Fortunately, efficient and flexible data management strategies for high performance computing have been successfully implemented in mesh based methods(eg. [12] for adaptive hp FEM, and [13], [14] for FVM). Motivated by techniques developed for mesh based methods, we present a complete framwork for parallelizing SPH program with MPI standard model allowing more flexible and efficient data access in this paper.
Any implementation of SPH code requires efficient searching and updating of neighbors during simulation. We adopted background grid which was proposed by Monaghan and Lattanzio [15] and implemented widespreadly in parallel SPH. The background grid is also used for domain decomposition in SPH. We refer to the elements of background grid, namely a squares for two dimension and cubics for three dimension, as buckets. As for the storage of physical quantities associated to each particle, different strategies was adopted in existing implementations of SPH. In both SPHysics [6] and DualSPHysics [9], The physical quantities of each particle (position, velocity, density) are stored in arrays, and the particles (and the arrays with particle data) are reordered following the order of the cells. This has two advantages: 1)access pattern is more regular and more efficient, 2) it is ease to identify the particles that belong to a cell by using a range since the first particle of each cell is known. But adding, deleting and especially accessing of particles are cumbersome. Angela Ferrari [7] adopted linked lists using pointers so that particles can be deleted or added during the simulation. Storage problems caused by fix-size arrays are thereby also eliminated. We define C++ classes which contains all data of particle and bucket. As for the management of data, we adopt an hash table to store pointers to particles and buckets, which gives us not only flexibility of deleting and adding element, but also quicker access compared with linked list. Instead of using the ”nature manner” to number particles, we adopt SFC based index to give each particle and background bucket an unique identifier. The SFC based numberring strategy is further extended to include time step information so that particles added at the same position but different time will have different identifiers. As for domain decomposion, even though more complicated graph-based partition tools [16] might get higher quality decomposition, they requires much more effort in programming. So we adopt an easy-programming scheme based on SFC [17].
To the best of the author’s knowledge, no implementation of SPH has the feature of adjusting computational domain based on simulation. For JPUE simulation, such feature will greatly reduce computational cost by avoiding computing of uninfluenced fluid. This feature is accomplished by adding a scan function to monitor the most outside layer of the domain and turn ghost particles to real particles at proper time.
The data structure, particle and bucket indexing strategies, domain decomposition , dynamic load balancing method and domain adjusting strategies in this paper can be easily adopted by other implementations of any meshfree methods(include SPH). The flexibility of data accessing enables implementing of meshless methods for solving of more complicated problems and using of more advanced techniques.

2. Data Structure and Load Balance

SPH is a meshfree, Lagrangian method. The domain is discretized by particles and the position of particle is updated at every time step. The physical laws (such as conservation laws of mass, momentum and energy) written in the form of partial differential equations need to be transformed into the Lagrangian formalism. Using a kernel function that provides the weighted estimate of the field variables at a discrete point (particle), the integral equations are evaluated as sums over neighbor particles. Only particles located within support of kernel function will interact. Thus, physical proterties (position, density, velocity, internal energy, pressure) are updated based on its neighbors. So a neighbor searching need to be carried out before updating of physical proterties. We use buckets which overlap the whole domain and keep fixed in time during the entire simulation, to reduce searching cost. Domain decomposition will be based on SFC going through centroids of all buckets. A basic works flow of our SPH code is shown in figure 1.
Particles need to be added and(or) removed during simulation of JPUE problems. Wall boundary conditions in SPH can be imposed either by adding a force term

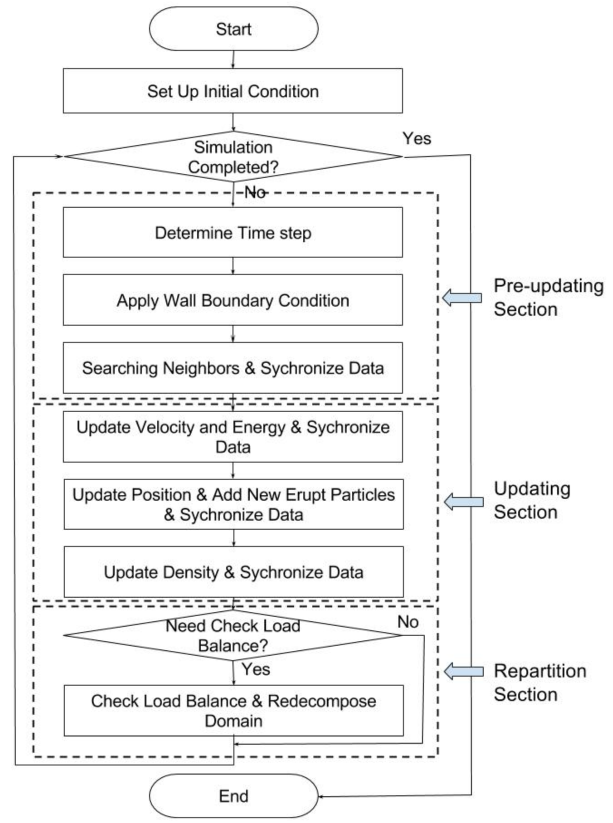

Start
Set Up Initial Condition
Simulation Completed?
Yes
No
Determine Time step
Apply Wall Boundary Condition
Searching Neighbors & Sychronize Data
Pre-updating Section
Update Velocity and Energy & Sychronize Data
Update Position & Add New Erupt Particles & Sychronize Data
Update Density & Sychronize Data
Updating Section
Need Check Load Balance?
No
Yes
Check Load Balance & Redecompose Domain
Repartition Section
End

Figure 1. Basic work flow for SPH

or using ghost particles. We adopt the latter one in our simulation. As our computational domain will be adjusted during simulation, wall ghost particles need to be added during simulation. New particles also need to be added for the eruption boundary condition. We will describe in this section these strategies which satisfies these demand.

2.1. SFC based indexing

Our data structure starts from assigning each particle and bucket an identifier, we refer to it as key, which should be unique throughout simulation. The key for a bucket is determined by centroid coordinates of the bucket while the key for a particle is determined by adding coordinates and adding time step of the particle. The map from coordinates to key is based on SFC.

The SFC [18] maps n-dimentional space to a one dimentional sequence. The standard procedure for obtainning SFC is:

- Scale coordinates into $[0, 1]^n$ based on maximum and minimum coordinates of the computational domain: $\mathbf{X}' \rightarrow \mathbf{X}$
- Compute $k_r = h_n(\mathbf{X})$. Where h_n is the map $h_n : [0, 1]^n \rightarrow [0, 1]$.
- Convert k_r to integer k by multiplying k_r with a very large number and removing decimal part.
- All keys are sorted to form a sequence which is SFC. The SFC represents a curve passing through all particles (or centroid of buckets).

Scheme for constructing the map h_n can be found in [19]. These keys denote a simple addressing/ordering scheme for the data and computations, i.e., a simple global index space for all the objects.

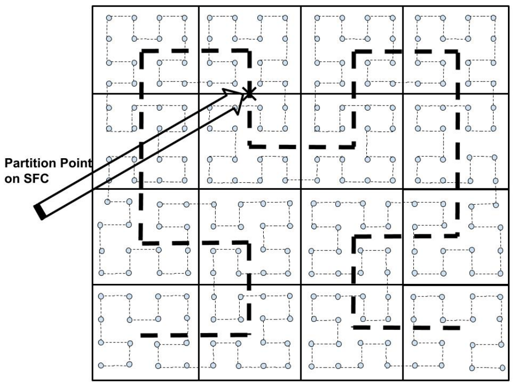
SFC-based indexing scheme can guarantee uniqueness of particle identifier only in simple scenarios when particles are added once while setting up initial condition. In some situations, new particles need to be added while simulation. For example, new particles need to be added at the bottom of the eject vent for JPUE simulation. To distinguish particles added at the "same place" (the small area, all points whithin which will be mapped to the same k.) at different time steps, we extend the SFC-based key to time-dependent SFC based key by including date of birth of particles into the key. The time-dependent SFC based key can be written as: $[k, t]$, where t is the time step. The map h_n will become:

$$h_n : [0, 1]^n \times \mathbf{T} \rightarrow [0, 1] \times \mathbf{N} \tag{1}$$

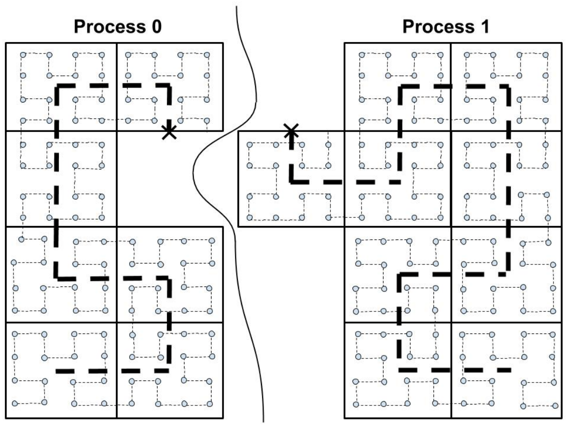
Where $\mathbf{T} \subset [0, \infty)$ is the time step dimension, $\mathbf{N} = \{0, 1, 2, 3...\}$. To guarantee locality, sorting of particle keys is majorly based on k, that is to say, particle with smaller k always comes before particles with larger k. For these particles have the same k, ordering of them will depend on t. Figure 2.1 shows SFC ordering of buckets and particles in buckets. Several features of such indexing scheme are suitable for SPH:

- Guarantee uniqueness of keys.
- Key of each object is generated purely based on its own coordinates. When add new objects on different processes, key of each object can be generated fast and independently.
- Objects that locate closely in the Euclidian space will also be close to each other in the one dimensional SFC key space in the mean sense. Since SPH particles only interact with its neighbors, geometric locality can be exploited for efficient storage and retrieval of bucket and particle data.
- This type of key effectivelly generate a global address space. Globality of key and conservation of locality make it easy to partition the sorted key squence and obtain the decompositiion of the problem.

What need emphasize here is that motion of particles might mess up locality that established based on ini-



(a) SFCs passing all particles and buckets



(b) Domain decomposition based on SFC of buckets

Figure 2. Spcace filling curve orderings of buckets and particles within the buckets

tial coordinates of particles. As particles are moving regularly, the locality of most of particles should still be conserved during simulation.

2.2. Data structure

2.2.1. Particle and bucket. The most basic data structure of SPH are particle, for problem discription, and bucket, for neighbors searching and domain decomposition. Both are defined as classes in C++. Infomation that contained in particle class can be categorized into six categorise: ID(the key), affiliate(rank of the process that the particle belongs to), primitive variables (variables show up as unknows in governing equations, eg. density, velocity, energy), secondary variables (properties that can be computed from primitive variables, they are stored to avoid repeatedly computing, eg. pressure, temperature ect.), flags (indicators, such as indicator for ghost particle and real particles, indicator for particles of different phases ect.) and neighbor infomation (it is a vector of particle keys in our application). Similarly, Infomation that contained in bucket class can also be categorized into different categorise: ID(the key), affiliate(rank of the process that the bucket belong to), domain information (maximum and mimnum coordinates, boundary infomation), flags (indicators, such as indicator for guest and non-guest, indicator for active and inactive), neighbor infomation (keys of 27 neighbor buckets for three dimension and keys of 9 neighbor buckets for two dimension including its own key) and possessed particles. Objects defined based on these two classes are then accesse through hash tables.

2.2.2. Hash table and hash confliction. As discussed at the beginning of this section, implementation of SPH in more realistic scenarios requires dynamic memory management and flexible data access. One of the fundemental data structures that satisfy such requirement is hash table. Another option is B-tree. We adopt hash table. An implementation of B-tree under a similar situation for mesh based methods can be found in other papers(eg. [20]).

Hash table, which is divided into slots, are array based data structure. Based on the key, the address-calculator(hashing) function determines in which slot the data should be stored. The hashing function maps from key to the slot index:

$$slot\,index = hash(key) \tag{2}$$

The hash table has O(1) data accessing, adding and deleting properties when there is no confliction. How many conflictions will happen depends on both distribution of keys in the key space and size of the hash table. As the distribution of keys is determined by particles' initial locations (or centroids of buckets), the hash table size is under our control. We can use very large hash table to minimize hash confliction on the expense of sparse data distribution which will lead to high cache missing and low memory efficiency. Or oppositely, we can use smaller hash table size to obtain high memory efficiency on the expense of having more hash conflictions. Abani [20] did numerical experiments to examine the effect of the table size on the dierent data management operations. One way to handle hash confliction is using an additional sorted vector attached to the hash table. When several keys hash to the same slot, a vector will be created. The vector is sorted based on keys so that a binary search can be used to find the correct position

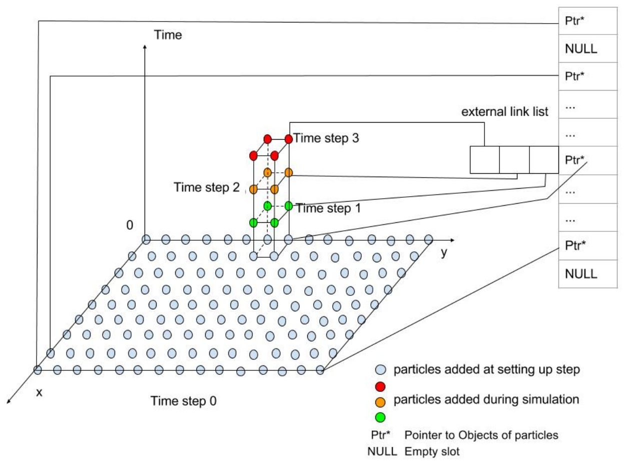

Time
Time step 3
Time step 2
Time step 1
Time step 0
external link list
0
x
y
Ptr*
NULL
...
particles added at setting up step
particles added during simulation
Ptr* Pointer to Objects of particles
NULL Empty slot

Figure 3. Ununiform distribution of particles in the $[0,1]^n \times \mathbf{T}$ space due to adding of new particles at a small portion of the domain, pointer to these new particles will be stored in external link list.

for adding, deleting or retrievaling . Another option to handle hash confliction is using an additional link list which is more flexible in memory allocation. The average time complexity of binary search is O(log n) while that for linear search based on link list is O(n). However, accessing efficiency of link list is much lower than array based data structure, especially when the link list becomes longger. Choosing of proper way to handle hash confliction greatly depends on the problem itself. For the test problem in this paper, successively adding of particles at the bottom of the eject vent will lead to hash confliction of many particles, which implies a long link list. But considering the very long conflictions only occur on several slots among millions (see figure 3), we still choose the link list to handle hash confliction. This decision was made based on numerical experiments.

2.2.3. Hash function. For time-independent keys, the hash function can be a simple function like:

$$Slot\,Index = \frac{Key - Min\,Key}{Max\,Key - Min\,Key} \times Hash\,Table\,Size \qquad (3)$$

One natural way to hash time-dependent SFC based key $[k, t]$ is to convert the two elements in the key into one number taking k as the higher digit and t as the lower digit of the large number. However, for JPUE simulation, even though ghost particles for wall boundary condition and pressure boundary condition

Table 1. Computational Cost Per Particle for Different Steps

Step	Cost (ms)	Abbreviation
neighbor search	0.41	NS
update momentum and energy	0.70	UPME
update density	0.42	UPD
update position	0.02	UPP
velocity filtering	0.43	VF
apply wall bc	0.75	WBC

Table 2. Computational Work Load for Each Type of Particle

Particle type	NS	UPME	UPD	UPP	VF	WBC	Total
Real	Yes	Yes	Yes	Yes	Yes	No	2.00
wall ghost	No	No	No	No	No	Yes	0.75
eruption ghost	No	No	No	Yes	No	No	0.02
pressure ghost	No	No	No	No	No	No	0.00

also need to be added during simulation, places for adding of these two types of ghost particles are previsouly empty area. Only ghost particles for eruption boundary condition will be successsively added at the same place: bottom of the vent. That is to say, particles are distributed ununiformly in the $[0,1]^n \times \mathbf{T}$ space as shown in figure 3. To avoid ununiform, very sparse hash table and conserve locality of SFC, we only plug the first number, k, of the key, $[k, t]$, into the hashing function, equation (3).

2.3. Load balancing strategy

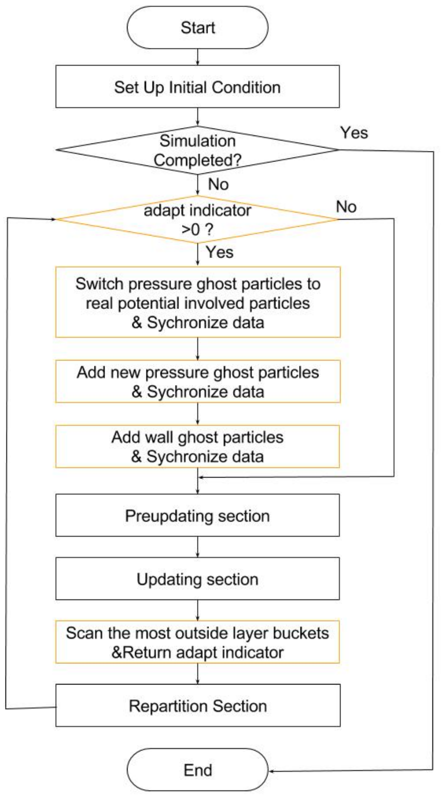
2.3.1. Weighted work load. Particles used in the test problem can be categorized into four types based the particle-type-flag: real particle, wall ghost particle, pressure ghost particle and eruption ghost particle. Ghost particles are for imposing of corresponding boundary conditions (see figure 3). As different types of particles involve different amount of computational work, shown by table 2 and table 1, we assign different work load weight for different types of particles based on profilling data. Instead of simply using number of contained particles as work load for bucket, work load of each bucket is determined by summing up work load weight of all particles within the bucket. The SFC sequence passing through centroids of all buckets now becomes a weighted sequence. Domain decomposition will conducted based on the weighted SFC of buckets.

2.3.2. Domain decomposition and dynamic load balancing. Domain decomposition will be conducted

based the weighted SFC of buckets. Figure 2 shows how domain is decomposed based on partition of SFC of buckets. The particles are automatically split into several groups along with buckets that contain them. As SFC of buckets is a curve in the three dimensional space, partition of this curve will automatically lead to 3D domain decomposition. A 2D domain decomposition based on SFC of footprint buckets projected by three dimensional buckets was adopted by Dinesh [8]. A comparision of the scalability of these two schemes (see figure 8) confirms that 3D domain decomposition is a better choice when processes number is larger. Movement of particles, adding of new particles, adjusting of domain will lead to important load imbalance between processes. To handle this, computational load is monitored at a given interval (The interval is optimized based on numerical experiments). And repartitioning is carried out when load imbalance is larger than a given tolerance.
As some of the neighbor particles reside in other partitions. A set of guest particles and buckets are used to synchronize data across partitions. To minimize communications, data is synchronized only where needed, using non-blocking MPI communications.

3. Adjusting of Domain During Simulation

As a Lagrangian method, SPH is able to automatically adjust computational domain as the postition of the dicretization points are updated at every time step. However, for JPUE simulation, where some fluid ejects into stationary fluid and get mixed due to turbulence, the domain-adjusting feature of SPH will gone. Because the whole domain, which occupied by stationary fluid before ejected fluid reaching there, has to be discretized at the very beginning of simulation. A lot of CPU time will be spent on computing of ”stationary” particles. It is pure wasting of computational resources. If simulating of stationary particls can be avoided, the computational cost will be reduced greatly. To the best of the author’s knowledge, no implementation of SPH has the feature of adjusting computational domain based on simulation. We propose a simple strategy to add such feature in our code with low computational cost. We add a scan function to monitor the most outside layer of the domain. When the ejected fluid reaches the boundary of the current domain, ghost particles (for pressure boundary condition) will be turn to real particles and then add new ghost particles for pressure boundary condition. The original work flow (see figure 1) is modified to enable such feature (see figure 4).
The start point of adding adjusting feature is adding


Start
Set Up Initial Condition
Simulation Completed?
Yes
No
adapt indicator >0 ?
No
Yes
Switch pressure ghost particles to real potential involved particles & Sychronize data
Add new pressure ghost particles & Sychronize data
Add wall ghost particles & Sychronize data
Preupdating section
Updating section
Scan the most outside layer buckets &Return adapt indicator
Repartition Section
End
Figure 4. Work flow that enables domain adjusting feature

a flag, which we refer to as involved-flag, into particle class. Particles are categorized into three groups based on the value of the involved-flag: involved (involved-flag=2), potential involved (involved-flag=1), and not involved(involved-flag=0). The involved particles are particles that have already been involved in eject mixing. The potential involved particles are particles that have not been involved in eject mixing but adjecent to involved particles. So they will be involved in the near future. These not involved particles are particles that far away from the eject source and are still at the initial state. For these not involved particles, it is meaningless to update its physical properties. As a consequence, searching for neighbors and data communitation for these particles are also unnecessary. That is to say, only potential involved and involved particles need to be simulated. As simulation goes, the ejected fluid will reach larger area and more and more particles will be influenced. When originally stationary air is influenced by erupted material, the mass fraction of the erupted material will increase from zero to a positive value. So we can determine whether a particle is involved or not based on whether the mass fraction of that particle is larger than a given threshold (10e-5 in our simulation). Other physical properties, such velocity, can also serve as alternative "swich criteria".

A has-involved-flag is added to bucket class, too. Buckets are then categorized into 3 types based on particles they contain: has involved (has-involved-flag=3), has potential involved(has-involved-flag=1) and has no involved (has-involved-flag=0). Bucket that has any involved particle will be set to be has involved (has-involved-flag=3). And its neighbor buckets that do not contain any involved particle will be set to be has potential involved. All particles in has involved buckets or has potential involved buckets will be set to be potential involved except for involved particles. There are two situations that will switch a has potential involved bucket to be a has involved bucket. First, when a involved particle enters a has potential involved bucket. Second, when mass fraction of a particle (It should be a potental involved particle) exceeds the threshold, this particle will turn to a involved particles and if this is the first involved particle in the bucket, the bucket will turn from a has potential involved bucket to a has involved bucekt.

The most outside buckets layer of all has potential involved buckets will be scaned every time after updating. If any of these buckets becomes has involved, the domain will be enlarged by turnning the pressure ghost particles to real particles and switching involved-flag from 0 to 1. Also, the buckets that originally contain pressure ghost particles will become has potential involved. New pressure ghost particles and wall ghost particles will be added around the adjusted domain. This domain adjusting process is shown in figure 5. The work flow with domain adjusting is in figure 4

For the test problem in this paper, the volcanic plume will finally reach to a region of $[-10km\ 10km] \times [-10km\ 10km] \times [0km\ 20km]$ after around 300 seconds of eruption. When numerical simulation goes up to 90 seconds, the plume is still within a region of $[-3km\ 3km] \times [-3km\ 3km] \times [0km\ 6km]$. This implies that adjusting of domain can avoid computing large number of uninfluenced air particles, especially for the beginning stage of simulation. Numercial test shows that simulation time of the test problem is reduce to $\frac{1}{4}$ of original simulation time when we adopt the domain adjusting strategy in our code.

4. Numerical Test

As we are targeting at developing data management and paralell strategies for more complicated implementations of SPH which demmand quick and flexible data access, delete and add. The test problem should have such demand. Volcanic eruption which is essentially a mutilple phases, turbulent, ejection mixing flow accompanied with microphysics processes requires more flexibile data management. We adopt a two phase volcanic plume model [21] as our test problem. In this model, one phase is air while another phase is ejected material.

4.1. Governing equations [21] and boundary conditions

Based on Navier-Stokes equations and several simplifications, the governing equations in Eulerian form are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{4}$$

$$\frac{\partial \rho \xi}{\partial t} + \nabla \cdot (\rho \xi \mathbf{v}) = 0 \tag{5}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v} + p\mathbf{I}) = \rho \mathbf{g} \tag{6}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + p)\mathbf{v}] = \rho \mathbf{g} \cdot \mathbf{v} \tag{7}$$

ξ is the mass fraction of ejected material. $E = e + K$ is total energy which is summation of kinetic energy K and internal energy e. An additional equation is required to close the system. In this model, the equation for closing the system is an EOS:

$$p = (\gamma_m - 1)\rho e \tag{8}$$

Where

$$\gamma_m = R_m / C_{vm} + 1 \tag{9}$$

$$Rm = n_g R_g + n_a R_a \tag{10}$$

$$C_{vm} = n_s C_{vs} + n_g C_{vg} + n_a C_{va} \tag{11}$$

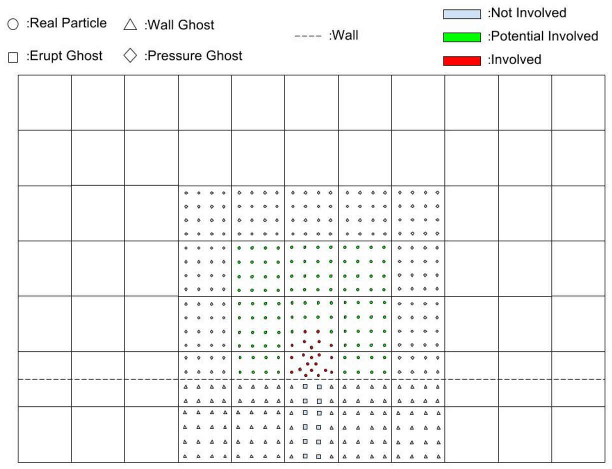
$$n_a = 1 - \xi \tag{12}$$

$$n_g = \xi n_{g0} \tag{13}$$

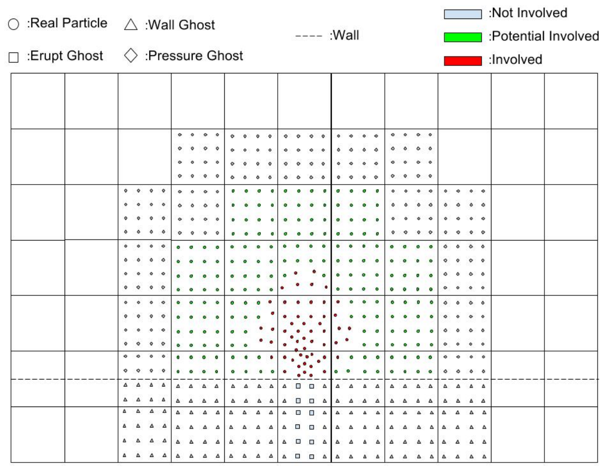
$$n_s = \xi - n_g \tag{14}$$

Where, C_v is specific heat with constant volume, n is mass fraction, R is gas constant. The subscription m represents mixture of ejected material and air, s is solid portion in ejected material, g is gas portion in the ejected material and a is air.

In current model the initial domain is a 3D box. The boundaries are categorized into eruption vent (a circle area at the center of the bottom), wall boundary (box bottom), pressure boundary (Other faces of the box). At the vent, T, $\mathbf{v} = \{0, 0, 150\}^T$, $p = 1.01 \times 10^5 Pa$, $n_{g0} = 0.05$ and mass discharge rate $\dot{M}$ is given. The radius of vent is determined from ρ, $\dot{M}$ and $\mathbf{v}$. Velocity is zero for non-slip wall boundary. We



(a) Computational domain at $t = t0$



(b) Computational domain at $t = t0 + \delta t$

Figure 5. Domain adjusting based on Involved flag of particles

assume the boundary to be adiabatic and the heat flux is zero on the bounday. The pressure of the surrounding atmosphere is specified on pressure boundaries. Except for the pressure, density, velocity, and energy will depend on the solution. We adpot ghost particles to impose these different type of boundary conditions (see figure 5).

4.2. Discretized governing equations with SPH

There are several review papers [22], [23], [24], [25], [26] which provide a pretty comprehensive view over SPH. We will not cover these basic theory of SPH in this paper. The discretized governing equations with SPH are:

$$< \rho_a^a >= \sum m_b w_{ab}(h_a) \tag{15}$$

$$< \rho_i^{sg} >= \sum_j m_j w_{ij}(h_i) \tag{16}$$

$$\begin{aligned} < \frac{d\mathbf{v}_\alpha}{dt} >= -\sum_b [m_b(\frac{p_b}{\rho_b^2} + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha b}) \\ \nabla_\alpha w_{\alpha b}(h_\alpha)] - \sum_j [m_j(\frac{p_j}{\rho_j^2} \\ + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha j}) \nabla_\alpha w_{\alpha j}(h_\alpha)] + \mathbf{g} \end{aligned} \tag{17}$$

$$\begin{aligned} < \frac{de_\alpha}{dt} >=0.5 \sum_b [m_b \mathbf{v}_{\alpha b}(\frac{p_b}{\rho_b^2} + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha b}) \\ \nabla_\alpha w_{\alpha b}(h_\alpha)] + 0.5 \sum_j [m_j \mathbf{v}_{\alpha b}(\frac{p_j}{\rho_j^2} \\ + \frac{p_\alpha}{\rho_\alpha^2} + \Pi_{\alpha j}) \nabla_\alpha w_{\alpha j}(h_\alpha)] \end{aligned} \tag{18}$$

Where ρ_a^a is density of phase 1 (air). ρ_i^{sg} is density of phase 2 (erupted material). $\rho = \rho^a + \rho^{sg}$ is density of mixture of phase 1 and phase 2.

$$\mathbf{v}_{\alpha b} = \mathbf{v}_\alpha - \mathbf{v}_b \tag{19}$$

$$\mathbf{v}_{\alpha j} = \mathbf{v}_\alpha - \mathbf{v}_j \tag{20}$$

$w_{ab}(h_a) = w(\mathbf{r}_a - \mathbf{r}_b, h_a)$ is smoothing kernel. Π is artificial viscosity term [22]. Index a, b is for phase 1. Index i, j is for phase 2. Index α, β can be index of either phase 1 or phase 2. The position of each particle is updated according to the following equation.

$$\frac{d\mathbf{r}_a}{dt} = \mathbf{v} \tag{21}$$

Free surface flow are in nature turbulent. We adopt $SPH - \varepsilon$ method developed by Monaghan [27] to capture turbulence in the plume. This will result to a filtered velocity for position updating and additional turbulent terms in momentum and energy eqution.

4.3. Solver performance

Experiments have been carried out on the computational cluster of Center for Computational Research (CCR) at Buffalo. The initial domain is $[-4800m, 4800m] \times [-4800m, 4800m] \times [0m, 6000m]$, with smoothing length (we set initial intervals between particles equal to smoothing length) equals to 200m and 100m respectively for test case1 and test case2. The computational work load of test case 2 is 8 times of that of the test case 1. The simulations run for 20s physical time. The consumed time and speed up are shows in figure 6 and 7. The results show linear

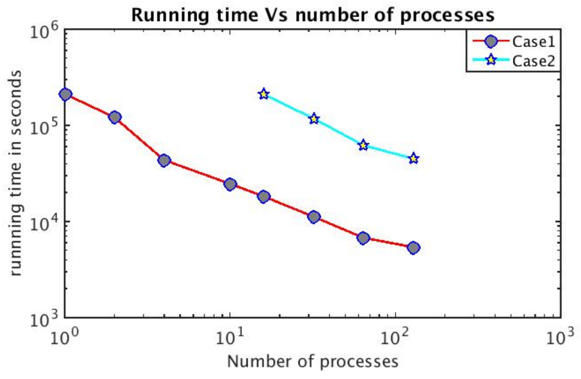


Figure 6. Excuting time of test case 1 and test case 2

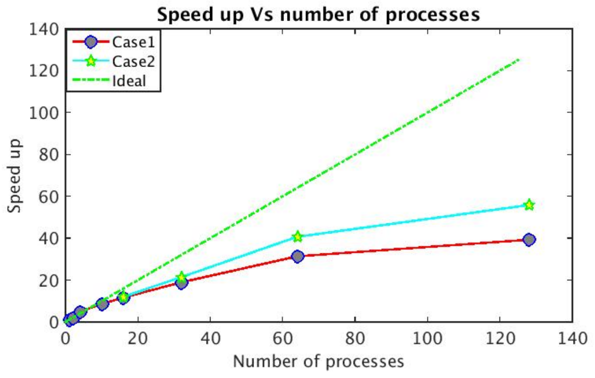


Figure 7. Influnece of total work load on strong scalability

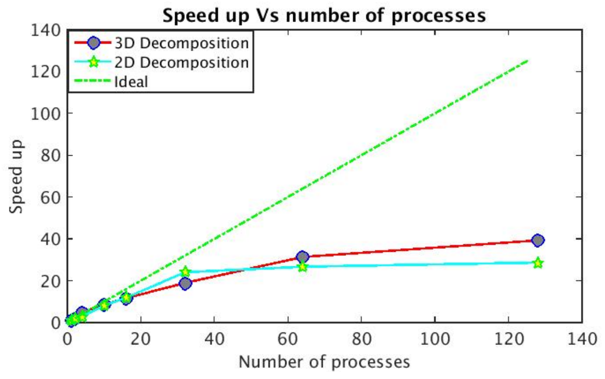


Figure 8. Strong scalability of 3D domain decomposition and 2D domain decomposition

speed up when number of processes is smaller than 16. The overhead of strong scalability can be increased by increasing total amount of work load which is demonstrated by the fact that test case2 has better speed up than test case1 when number of processes is larger. We also compared the performance of 2D domain decomposition and 3D domain decomposition. As shown by figure 8, 2D domain decomposition shows a little bit better strong scalability than 3D domain decomposition for number of processes is 32. When number of processes is 64 and 128, 3D domain decomposition shows a better speed up. That is because the total number of footprint buckets in x-y plane is 64 in the test case. When we request 128 processes, 64 processes will be totally idle at the beginning. As simulation goes, the domain will expand and more and more idle processes will start getting tasks. That's why we still get some speed up when number of process is 128. 3D domain decomposition is able to divide the work load in a more flexible way and achieve better strong scalability.

5. Conclusion

We developed data management strategies for parallel implementation of SPH method using MPI standard to simulate complicated problems, such as JUPE, which requires flexible and fast data retrievalling, adding and deleting. Neighbors searching and domain decomposition is based on background grid which overlaps the domain and keep stationary during simulation. SFC based index scheme, which provides a global numberring methodology that is purely coordinates dependent, is adopted to give each bucket an unique identifier. A time dependent key which is also based on SFC is used as identifier for particles. Hashtables with external link list are adopted for accessing particles and buckets data. Based on weighted particle work load, a dynamic load balance strategy is developed by checking load balance and redecomposing the domain at an optimize interval. The code was further improved to 4 times faster by adjusting computational domain according to progress of simulation. Performance tests on our code shew a linear speed up and an overhead cast by total among of work load. 3D domain decomposition has better scalability than 2D domain decomposition when number of processes is larger.

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